4. Topological phases-a

In this chapter we try to learn various topological phases and understand what topological properties can arise for free fermion systems subject to some symmetry constraints.

Tight-binding models

We assume that the system is a discrete lattice and electrons can only stay on the lattice site. The kinetic energy is included by allowing electrons to hop from one site to another.

1. A one-band model

Let's consider a 1D lattice with one atom per unit cell. For each atom, we consider only one quantum state. The creation (annihilation) operator $c_i^\dagger (c_i)$ creates and annihilates one particle on site i. The non-interacting Hamiltonian can be written as

$$H = -\sum_{ij} \left(t_{ij} c_i^\dagger c_j + t_{ji} c_j^\dagger c_i \right) + \sum_i V_i c_i^\dagger c_i$$

The first term $\sum_{ij} t_{ij} c_i^\dagger c_j$ describes hoppings from site j to i. The second term $\sum_{ij} t_{ji} c_j^\dagger c_i$ describes the hopping from i to j. The last term is the potential energy. Because the lattice contains only one type of atoms, V_i = constant. Because H is Hermitian, we find that $t_{ij} = t_{ji}^*$ and V_i is a real number.

Proof:

$$H^\dagger = H$$

$$\left[-\sum_{ij} \left(t_{ij} c_i^\dagger c_j + t_{ji} c_j^\dagger c_i \right) + \sum_i V_i c_i^\dagger c_i \right]^\dagger$$

$$= -\sum_{ij} \left(t_{ij} c_i^\dagger c_j + t_{ji} c_j^\dagger c_i \right) + \sum_i V_i c_i^\dagger c_i - \sum_{ij} \left(t_{ij}^* c_j^\dagger c_i + t_{ji} c_i^\dagger c_j \right) + \sum_i V_i^* c_i^\dagger c_i$$

$$= -\sum_{ij} \left(t_{ij} c_i^\dagger c_j + t_{ji} c_j^\dagger c_i \right) + \sum_i V_i c_i^\dagger c_i$$

By comparing the two sides, we find that $t_{ij}^* = t_{ji}$ and $V_i = V_i^*$.

Therefore, we can simplify the Hamiltonian

$$H = -\sum_{ij} \left(t_{ij} c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i \right) + V \sum_i c_i^\dagger c_i = -\sum_{ij} \left(t_{ij} c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i \right) + VN$$

In the last term, $N = \sum_i c_i^\dagger c_i$ is the total number of electrons in the system. Because VN is a constant, this term just shifts the total energy by a constant, and thus has no other physical contribution.

Due to the translational symmetry, all nearest-neighbor hoppings shall have the same hopping strength. If we assume that this hopping strength is a real number t, the Hamiltonian is

$$H = -t\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) = -t\sum_i c_i^\dagger c_{i+1} + h.c.$$

Here, $\langle ij\rangle$ implies that i and j must be neighbors. On the right-hand side, $h.c.$ means Hermitian conjugate.

Fourier series: We have a continuous k-space and it is periodic (the Brillouin zone), but the real space is discrete.

$$c_k = \frac{1}{\sqrt{2\pi/a}}\sum\nolimits_i c_i e^{-ikx}$$

$$c_i = \frac{1}{\sqrt{2\pi/a}}\int_{BZ} c_i e^{ikx}$$

Because $\{c_i, c_j^\dagger\} = \delta_{ij}$, it is easy to check that

$$\begin{aligned}\{c_k, c_{k'}^\dagger\} &= \left\{\frac{1}{\sqrt{2\pi/a}}\sum\nolimits_i c_i e^{-ikx_i}, \frac{1}{\sqrt{2\pi/a}}\sum\nolimits_j c_j^\dagger e^{ik'x_j}\right\} = \sum\nolimits_{i,j}\{c_i, c_j^\dagger\}\frac{1}{2\pi/a}e^{-ikx_i}e^{ik'x_j}\\ &= \sum\nolimits_{i,j}\delta_{ij}\frac{1}{2\pi/a}e^{-i(k-k')x_i} = \sum\nolimits_i \frac{1}{2\pi/a}e^{-i(k-k')ia} = a\delta\big((k-k')a\big)\\ &= \delta(k-k')\end{aligned}$$

If we know $\{c_k, c_{k'}^\dagger\} = \delta(k-k')$, we can also show that $\{c_i, c_j^\dagger\} = \delta_{ij}$.

$$\begin{aligned}\{c_i, c_j^\dagger\} &= \left\{\frac{1}{\sqrt{2\pi/a}}\int_{BZ} dk c_k e^{ikx_i}, \frac{1}{\sqrt{2\pi/a}}\int_{BZ} dk' c_{k'}^\dagger, e^{-ik'x_j}\right\}\\ &= \frac{1}{2\pi/a}\int_{BZ} dk\int_{BZ} dk'\,\delta(k-k')e^{ikx_i}e^{-ik'x_j} = \frac{1}{2\pi/a}\int_{BZ} dk\, e^{ik(x_i-x_j)} = \delta_{ij}\end{aligned}$$

Hamiltonian in k-space. We can transfer the Hamiltonian into the k-space. In real space, it looks like

$$H = -t\sum_i c_i^\dagger c_{i+1} + h.c.$$

The first term is

$$\sum_j c_j^\dagger c_{j+1} = \sum_j \frac{1}{\sqrt{2\pi/a}} \int_{BZ} dk c_k^\dagger e^{-ikaj} \frac{1}{\sqrt{2\pi/a}} \int_{BZ} dk' c_{k'}^\dagger e^{ik'(j+1)a}$$

$$= \sum_j \frac{1}{2\pi/a} \int_{BZ} dk \int_{BZ} dk' c_k^\dagger c_{k'} e^{ik'a} e^{-i(k'-k)aj}$$

$$= \int_{BZ} dk \int_{BZ} dk' c_k^\dagger c_{k'} e^{ik'a} \delta(k-k') = \int_{BZ} dk\, c_k^\dagger c_k e^{ika}$$

The second term is the Hermitian conjugate of the first term, so

$$h.c. = \left(\sum_j c_j^\dagger c_{j+1} \right)^\dagger = \left(\int_{BZ} dk\, c_k^\dagger c_k e^{ika} \right)^\dagger = \int_{BZ} dk\, c_k^\dagger c_k e^{-ika}$$

$$H = -t \sum_i c_i^\dagger c_{i+1} + h.c. = -t \int_{BZ} dk\, c_k^\dagger c_k e^{ika} - t \int_{BZ} dk\, c_k^\dagger c_k e^{-ika} = -2t \int_{BZ} dk\, c_k^\dagger c_k \cos ka$$

$$= \int_{BZ} dk\, (-2t \cos ka) c_k^\dagger c_k$$

For a solid, we know that the total energy of electrons (ignore interactions) is

$$E = \sum\nolimits_n \int_{BZ} dk \epsilon_n(k) n_n(k)$$

where the summation sums over all bands, $\epsilon_n(k)$ is the dispersion relation for band n and $n_n(k)$ is the occupation number for the Bloch wave state in band n with momentum k. In second quantization,

$$H = \sum\nolimits_n \int_{BZ} dk \epsilon_n(k) \gamma_{n,k}^\dagger \gamma_{n,k}$$

Here, $\gamma_{n,k}^\dagger$ is the creation operator for a Bloch wave $\psi_{n,k}(r) = u_{n,k} e^{ikr}$. If we compare this formula with the tight-binding Hamiltonian (in k space), we find immediately that the tight-binding model we considered here has only one energy band. And our $c_k^\dagger$ operator is in fact the creation operator for Bloch waves. And the dispersion relation for this band is $\epsilon_k = -2t \cos ka$. Notice that ϵ_k is a periodic function of k with periodicity $2\pi/a$, which is exactly what we expect for Bloch waves.

Discrete Fourier transformation and Fourier series

Here, we briefly discuss about the discrete Fourier transform. Consider a discrete function f_i, where i = 1, 2, 3…N marks different lattice site. In addition, we assume the periodic boundary condition $f_{N+i} = f_i$. We can define

$$\tilde{f}_k = \frac{1}{\sqrt{N}} \sum_j f_j e^{-ikaj}$$

where a is the lattice constant and j marks the different lattice sites. And it's easy to prove that

$$f_j = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k e^{ikaj}$$

Same as j, the wave vector k here is also a discrete variable. This is because $f_{N+i} = f_N$ (our system has a finite size)

$$f_{j+N} = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k e^{ik(aj+aN)} = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k e^{ikaj}\, e^{ikaN}$$

$$f_j = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k e^{ikaj}$$

If we compare the two equations, we find that $e^{ikaN} = 1$, which implies

$$k = \frac{2\pi m}{\sqrt{N}} = \frac{2\pi m}{L}$$

Here $L = Na$ is the size of the system. For infinite systems, $L \to \infty$, the discrete sum Σ_k turns into an integral $\int dk$.

Same as j, k also have a periodicity, and the periodicity is also N. This periodicity is just the Brillouin zone.

Define $k_m = \frac{2\pi m}{L}$ and by definition,

$$\tilde{f}_{k_m} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-ik_m aj} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-i\left(\frac{2\pi}{Na}m\right)aj} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-i\frac{2\pi}{N}j}$$

For k_{m+N}, by definition

$$\tilde{f}_{k_{m+N}} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-ik_{m+N}aj} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-i\left[\frac{2\pi}{Na}(m+N)\right]aj} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-i\frac{2\pi}{N}mj}\, e^{-i2\pi j}$$

Because j is an integer, the factor $e^{-i2\pi j} = 1$. Therefore

$$\tilde{f}_{k_{m+N}} = \frac{1}{\sqrt{N}} \sum_j f_j e^{-i\frac{2\pi}{N}mj} = \tilde{f}_{k_m}$$

As a result, we can limit the value of m to be $-N/2 \leq m < N/2$. If m is not in this range, the value of $\tilde{f}_{k_m}$ can be obtained using the periodic condition $\tilde{f}_{k_{m+M}} = \tilde{f}_{k_m}$

$$m = -\frac{N}{2}, -\frac{N}{2}+1, \dots, \frac{N}{2}-1,$$

For the wave vector k, this means that

$$\tilde{f}_{k+2\pi/a} = \tilde{f}_k$$

So, we can confine the value of k into the range of $\pi/a \leq k < \pi/a$, which is the first Brillouin zone. For k outside the first Brillouin zone, we can find the corresponding $\tilde{f}_k$ using the periodicity $\tilde{f}_{k+2\pi/a} = \tilde{f}_k$

$$k = -\frac{\pi}{a}, -\frac{\pi}{a}+1\times\frac{2\pi}{L}, -\frac{\pi}{a}+2\times\frac{2\pi}{L}, \dots, \frac{\pi}{a}-1\times\frac{2\pi}{L}$$

Two useful Identities:

$$\frac{1}{N}\sum\nolimits_k e^{ikaj}\, e^{-ikaj'} = \delta_{j,j'}$$

$$\frac{1}{N}\sum\nolimits_j e^{ikaj}\, e^{-ik'aj} = \delta_{k,k'}$$

Therefore, in a one-band model, the eigenvector is trivial, which is just identity. Therefore, the Berry $\vec{\mathcal{A}}_n = -i\int dx\left[u_{n,k}(x)\right]^* \nabla_{\vec{k}}\, u_{n,k}(x)$ must be trivial $\vec{\mathcal{A}}_n = 0$. This tells us that a one-band model can never show quantum Hall effect. We need at least two bands. In fact, one can prove that the total Chern number summing over all bands must be zero.

2. A two-band model in 1D

Let us consider a 1d chain formed by two different types of atoms (a and b). For each atom, we consider only one quantum state. The non-interacting Hamiltonian can be written as

$$H = -t\sum_i \left(a_i^\dagger b_i + b_i^\dagger a_{i+1} + h.c.\right) + V_a\sum_i a_i^\dagger a_i + V_b\sum_i b_i^\dagger b_i$$

Here, the position of a sites in the jth unit cells is $r = a\times j + r_a$, and the position of b sites in the jth unit cells is $r = a\times j + r_b$, where a is the lattice constant (the size of a unit cell). The creation (annihilation) operator $a_i^\dagger, b_i^\dagger (a_i, b_i)$ creates and annihilates one particle on site i for atom a, b.

The first sum describes hopping from site b_i to a_i and a_{i+1} to b_i. $h.c.$ means Hermitian conjugate of the first term, so we just use $h.c.$ to represent it.

The second and third sums are the potential energies, $\sum_i \ a_i^\dagger a_i$ and $\sum_i \ b_i^\dagger b_i$ are the total numbers of electrons in *a* sites and *b* sites.

Discrete Fourier series. Both the site i and wave vector k are discrete variables.

$$a_k = \frac{1}{\sqrt{N}} \sum_i a_i e^{ikx}$$

$$a_i = \frac{1}{\sqrt{N}} \sum_k a_k e^{-ikx}$$

$$b_k = \frac{1}{\sqrt{N}} \sum_i b_i e^{ikx}$$

$$b_i = \frac{1}{\sqrt{N}} \sum_k b_k e^{-ikx}$$

Hamiltonian in k-space. By using these Fourier series, we can transfer the Hamiltonian into the k-space

$$\begin{aligned}\sum_j a_j^\dagger b_j &= \sum_j \frac{1}{\sqrt{N}} \sum_k a_k^\dagger e^{-ik(aj+r_a)} \frac{1}{\sqrt{N}} \sum_{k'} b_{k'} e^{ik'(aj+r_b)} \\ &= \frac{1}{N} \sum_k \sum_{k'} a_k^\dagger b_{k'} \sum_j e^{-ik(aj+r_a)} e^{ik'(aj+r_b)} \\ &= \sum_k \sum_{k'} a_k^\dagger b_{k'} \frac{1}{N} \sum_j e^{-i(k-k')aj} e^{-ik'r_a} e^{ik'r_b} = \sum_k a_k^\dagger b_k e^{ik(r_b-r_a)}\end{aligned}$$

In k-space, hoppings from *b* to *a* result in a term in Hamiltonian $\sim \sum_k \ a_k^\dagger b_k e^{ik(r_b-r_a)}$. The phase factor here is determined by how far the electron hop, i.e. $r_b - r_a$. We apply the same conclusion to the hopping from *a* to *b*

$$\sum_j b_j^\dagger a_{j+1} = \sum_k b_k^\dagger a_k e^{ik(r_a-r_b)}$$

If $r_b - r_a = a/2$,

$$\sum_j a_j^\dagger b_j = \sum_k a_k^\dagger b_k e^{ika/2}$$

$$\sum_j b_j^\dagger a_{j+1} = \sum_k b_k^\dagger a_k e^{ika/2}$$

For the potential term, we also know that

$$\sum_i a_i^\dagger a_i = \sum_k a_k^\dagger a_k, \quad \sum_i b_i^\dagger b_i = \sum_k b_k^\dagger b_k$$

Therefore, in the k-space

$$H = -t\sum_k \left(a_k^\dagger b_k e^{\frac{ika}{2}} + b_k^\dagger a_k e^{\frac{ika}{2}} + b_k^\dagger a_k e^{-\frac{ika}{2}} + a_k^\dagger b_k e^{-\frac{ika}{2}}\right) + V_a\sum_k a_k^\dagger a_k + V_b\sum_k b_k^\dagger b_k$$

$$-2t\sum_k \left[\left(a_k^\dagger b_k \cos\left(\frac{ka}{2}\right) + b_k^\dagger a_k \cos\left(\frac{ka}{2}\right)\right) + V_a a_k^\dagger a_k + V_b b_k^\dagger b_k\right]$$

We can further write it in a matrix form:

$$H = \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \mathcal{H}(k) \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

where $\mathcal{H}$ is a 2x2 Hermitian matrix. It is called the kernel of the Hamiltonian. The Hamiltonian H must be gauge invariant, but $\mathcal{H}(k)$ is not. For example, if we change $a^\dagger \to a^\dagger e^{i\phi}$, the Hamiltonian H is invariant, but the kernel $\mathcal{H}(k)$ is NOT.

For the model considered here,

$$\mathcal{H}(k) = \begin{pmatrix} V_a & -2t\cos\left(\frac{ka}{2}\right) \\ -2t\cos\left(\frac{ka}{2}\right) & V_b \end{pmatrix}$$

For more generic cases, if one has m quantum states per unit cell, $\mathcal{H}(k)$ will be a m×m Hermitian matrix.

In the following, we will discuss the physical meanings of the eigenvalues and eigenvectors of $\mathcal{H}(k)$.

Eigenvalues of the kernel: The eigenvalues of $\mathcal{H}(k)$ give us the dispersion relations. At each k point, one can define a unitary transformation

$$\begin{pmatrix} c_k \\ d_k \end{pmatrix} = U_k^{-1} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

$$\begin{pmatrix} c_k^\dagger & d_k^\dagger \end{pmatrix} = \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} U_k$$

where $U_k^{-1} = U_k^\dagger$. So

$$H = \sum_k \begin{pmatrix} c_k^\dagger & d_k^\dagger \end{pmatrix} U_k^\dagger \mathcal{H} U_k \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

If we choose U_k such that $U_k^\dagger \mathcal{H} U_k$ is a diagonal matrix,

$$U_k \mathcal{H} U_k^{-1} = \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix}$$

Then, the Hamiltonian becomes

$$H = \sum_k \begin{pmatrix} c_k^\dagger & d_k^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix} = \sum_k \epsilon_c(k) c_k^\dagger c_k + \sum_k \epsilon_d(k) d_k^\dagger d_k$$

We know that using Bloch waves (which are eigenstates of the Hamiltonian), the total energy is

$$E = \sum_{k,m} \epsilon_m(k)\, n_m(k) = \sum_k \epsilon_1\, n_1(k) + \sum_k \epsilon_2\, n_2(k) + \sum_k \epsilon_3\, n_3(k) + \cdots$$

where $\epsilon_m(k)$ is the dispersion relation for the mth band and $n_m(k)$ is the occupation number for the quantum state in the mth band with momentum k. Therefore, in terms of Bloch waves:

$$H = \sum_k \epsilon_1\, \gamma_{1,k}^\dagger \gamma_{1,k} + \sum_k \epsilon_2\, \gamma_{2,k}^\dagger \gamma_{2,k} + \sum_k \epsilon_3\, \gamma_{3,k}^\dagger \gamma_{3,k} + \cdots$$

where $\gamma_{n,k}^\dagger$ is the creation operator for a Bloch wave in band n at momentum k. If we compare this formula with the equation at two lines above, we find that in this model we get two energy bands. $c_k^\dagger$ creates a Bloch wave with momentum k in one of the bands. $d_k^\dagger$ creates a Bloch wave with momentum k in the other band. For the bands created by $c_k^\dagger$, its dispersion relation is $\epsilon_c(k)$, while the other hand has a dispersion relation $\epsilon_d(k)$.

For the problem we considered here, the dispersions are

$$\epsilon_c = \frac{V_a + V_b}{2} - \sqrt{\left[2t\cos\left(\frac{ka}{2}\right)\right]^2 + \left(\frac{V_a - V_b}{2}\right)^2}$$

$$\epsilon_d = \frac{V_a + V_b}{2} + \sqrt{\left[2t\cos\left(\frac{ka}{2}\right)\right]^2 + \left(\frac{V_a - V_b}{2}\right)^2}$$

which are the eigenvalues of the matrix $\mathcal{H}(k)$.

If we have a model with m orbitals per unit cell, $\mathcal{H}(k)$ would be a $m \times m$ matrix. This matrix will have m eigenvalues, which results in a m-band model and each eigenvalue $\epsilon_n(k)$ is the dispersion relation for one of the bands.

Eigenvectors of $\mathcal{H}(k)$

The eigenvectors of $\mathcal{H}(k)$ give us the Bloch waves. The two-by-two matrix $\mathcal{H}(k)$ has two eigenvalues, $\epsilon_c(k)$ and $\epsilon_d(k)$. For each eigenvalue, the corresponding eignevector is a 2-component vector:

$$\mathcal{H}\begin{pmatrix} v_a^{(-)}(k) \\ v_b^{(-)}(k) \end{pmatrix} = \epsilon_c \begin{pmatrix} v_a^{(-)}(k) \\ v_b^{(-)}(k) \end{pmatrix}$$

$$\mathcal{H}\begin{pmatrix} v_a^{(+)}(k) \\ v_b^{(+)}(k) \end{pmatrix} = \epsilon_d \begin{pmatrix} v_a^{(+)}(k) \\ v_b^{(+)}(k) \end{pmatrix}$$

It can be easily checked that

$$c_k^\dagger = v_a^{(-)}(k) a_k^\dagger + v_b^{(-)}(k) b_k^\dagger$$

$$d_k^\dagger = v_a^{(+)}(k) a_k^\dagger + v_b^{(+)}(k) b_k^\dagger$$

We know that $a^\dagger$ and $b^\dagger$ are the creation operators for plane waves and we also know that $c_k^\dagger$ and $d_k^\dagger$ create Bloch waves. The relation between plane waves and Bloch waves is

$$\psi_{n,k}(x) = u_{n,k}(x) \frac{e^{ikx}}{\sqrt{N}}$$

So, the coefficients $v_a^{(\pm)}(k)$ and $v_b^{(\pm)}(k)$ here are in fact the discrete version of $u_{n,k}(x)$. **The eigenvectors of $\mathcal{H}(k)$ give us the Bloch waves $u_{n,k}$.**

We have learned that the Berry connection $\mathcal{A}_n(\mathrm{k})$ is defined as

$$\vec{\mathcal{A}}_n = -i\langle u_{n,k} | \nabla_{\vec{k}} | u_{n,k} \rangle$$

For continuous models, this formula means

$$\vec{\mathcal{A}}_n = -i \int dx \left[u_{n,k}(x)\right]^* \nabla_{\vec{k}} u_{n,k}(x)$$

For lattice models (tight-binding models)

$$\vec{\mathcal{A}}_- = -i\begin{pmatrix} v_a^{(-)}(k)^* & v_b^{(-)}(k)^* \end{pmatrix} \nabla_{\vec{k}} \begin{pmatrix} v_a^{(-)}(k) \\ v_b^{(-)}(k) \end{pmatrix}$$

$$\vec{\mathcal{A}}_+ = -i\begin{pmatrix} v_a^{(+)}(k)^* & v_b^{(+)}(k)^* \end{pmatrix}\nabla_{\vec{k}}\begin{pmatrix} v_a^{(+)}(k) \\ v_b^{(+)}(k) \end{pmatrix}$$

In general, for a m band model, where $\mathcal{H}(k)$ is a $m \times m$ matrix, each of the eigenvector gives us the Bloch wavefunction for one of the m bands. We can use each eigenvector to compute the Berry connection, the Berry curvature and the Chern number for that band.

Summary

- The key properties of a tight-binding model are coded in $\mathcal{H}(k)$, which is a $m \times m$ Hermitian matrix. Each component is a function of k. (In other words, $\mathcal{H}(k)$ is a matrix function of k.)
- The eigenvalues if $\mathcal{H}(k)$ gives the band structure (the dispersion relation) for each bands $\epsilon_n(k)$ with n = 1, 2, …m
- The eigenvectors as a function of k gives the Bloch wave: $u_{n,k}(\alpha)$, where n=1,2,…, m is the band index and α =1,2…m marks different site in a unit cell.
- Using these $u_{n,k}(\alpha)$, we can define the Berry connection, Berry curvature and the Chern number. Just replace the integral in the real space by summing over α =1,2…m

Although the wavefunction cannot be measured directly, it contains the topological information, which is a physical observable (e.g. the Hall conductivity).

3. An example of a topologically nontrivial insulator (Qi-Wu-Zhang model, Half BHZ model)

Let's consider a two-band model, whose kernel is

$$\mathcal{H}(k) = \begin{pmatrix} -2t\cos k_x - 2t\cos k_y - \mu & \Delta(\sin k_x - i\sin k_y) \\ \Delta(\sin k_x + i\sin k_y) & 2t\cos k_x + 2t\cos k_y + \mu \end{pmatrix}$$

Here we assume $\Delta > 0$ and $t > 0$ and $-4|t| < \mu < 4|t|$. In real space, this Hamiltonian corresponds to a square lattice and on each site there are two quantum states. Please notice that here μ refers to a control parameter, which is NOT the chemical potential.

Two-band models and Pauli matrices

For any two-band models, $\mathcal{H}$ is a two-by-two Hermitian matrix. For a two-by-two Hermitian matrix, one can always separate it into the identity and Pauli matrices I, and σ_i

$$\mathcal{H} = \mathcal{H}_0(k)I + \mathcal{H}_x(k)\sigma_x + \mathcal{H}_y(k)\sigma_y + \mathcal{H}_z(k)\sigma_z$$

where $\mathcal{H}_0(k)$, $\mathcal{H}_x(k)$, $\mathcal{H}_y(k)$, and $\mathcal{H}_z(k)$ are real function of k. If we define $\mathcal{H}(k) = \left(\mathcal{H}_x(k), \mathcal{H}_y(k), \mathcal{H}_z(k)\right)$, we find that

$$\mathcal{H} = \mathcal{H}_0(k)I + \vec{\mathcal{H}}(k)\cdot\vec{\sigma}$$

This Hamiltonian is rather similar to a spin under magnetic fields $H = -\vec{B}\cdot\vec{\sigma} + B$

For the case studied here,

$$\mathcal{H}_0(k) = 0$$

$$\mathcal{H}_x(k) = \Delta\sin k_x$$

$$\mathcal{H}_y(k) = \Delta\sin k_y$$

$$\mathcal{H}_z(k) = -2t\cos k_x - 2t\cos k_y - \mu$$

The eigenvalues of $\mathcal{H}$ are

$$E_\pm = \mathcal{H}_0(k) \pm |\mathcal{H}(k)| = \mathcal{H}_0(k) \pm \sqrt{\mathcal{H}_x(k)^2 + \mathcal{H}_y(k)^2 + \mathcal{H}_z(k)^2}$$

This is pretty much the same as the spin system, where the eigen-energies of the are $= B \pm \left|\vec{B}\right| = 0$ or $2B$.

For a two-band model, the top band has energy $E_+ \geq \mathcal{H}_0$, while the lower band has $E_- \leq \mathcal{H}_0$. The energy gap between the two bands is:

$$\Delta(k) = E_+ - E_- = 2\left|\vec{\mathcal{H}}(k)\right|$$

As long as $\left|\vec{\mathcal{H}}(k)\right| \neq 0$, the two band will not cross with each other. Let's now focus on the lower band E_-), its eigenvector is

$$u_-^{(I)}(k) = \frac{1}{N^{(I)}}\begin{pmatrix}\mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\mathcal{H}_y(k)\end{pmatrix}$$

This is indeed a problem for the Hamiltonian shown above. At $k_x = k_y = \pi$.

$$\mathcal{H}_0(k) = 0$$

$$\mathcal{H}_x(k) = \Delta\sin k_x = 0$$

$$\mathcal{H}_y(k) = \Delta\sin k_y = 0$$

$$\mathcal{H}_z(k) = -2t\cos k_x - 2t\cos k_y - \mu = 4t - \mu > 0$$

Remember that we assumed $|\mu| < 4t$. In fact, there is another way to write down the same eigenvector (i.e. a phase shift)

$$u_{-}^{(II)}(k)=\frac{1}{N^{(I)}}\begin{pmatrix}\mathcal{H}_z(k)-\left|\vec{\mathcal{H}}(k)\right|\\ \mathcal{H}_x(k)+i\mathcal{H}_y(k)\end{pmatrix}\times\frac{\frac{\mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k)+i\mathcal{H}_y(k)}}{\left|\frac{\mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k)+i\mathcal{H}_y(k)}\right|}=\frac{1}{N^{(II)}}\begin{pmatrix}\frac{-\mathcal{H}_x(k)^2-\mathcal{H}_y(k)^2}{\mathcal{H}_x(k)+i\mathcal{H}_y(k)}\\ \mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|\end{pmatrix}$$
$$=\frac{1}{N^{(II)}}\begin{pmatrix}-\mathcal{H}_x(k)+i\mathcal{H}_y(k)\\ \mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|\end{pmatrix}$$

The two wavefunction $u_{-}^{(I)}(k)$ and $u_{-}^{(II)}(k)$ differ by a phase

$$u_{-}^{(II)}(k)=u_{-}^{(I)}(k)e^{i\phi(k)}$$

where

$$e^{i\phi(k)}=\frac{\frac{\mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k)+i\mathcal{H}_y(k)}}{\left|\frac{\mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k)+i\mathcal{H}_y(k)}\right|}$$

This new wavefunction is well defined at $\mathcal{H}_x(k)=\mathcal{H}_y(k)=0$ and $\mathcal{H}_z(k)>0$:

$$u_{-}^{(II)}(k)=\frac{1}{N^{(II)}}\begin{pmatrix}-\mathcal{H}_x(k)+i\mathcal{H}_y(k)\\ \mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|\end{pmatrix}=\frac{1}{N^{(II)}}\begin{pmatrix}0\\ 2\mathcal{H}_z(k)\end{pmatrix}$$

However, it is NOT well defined at $\mathcal{H}_x(k)=\mathcal{H}_y(k)=0$ and $\mathcal{H}_z(k)<0$. There, we find

$$u_{-}^{(II)}(k)=\frac{1}{N^{(II)}}\begin{pmatrix}-\mathcal{H}_x(k)+i\mathcal{H}_y(k)\\ \mathcal{H}_z(k)+\left|\vec{\mathcal{H}}(k)\right|\end{pmatrix}=\frac{1}{N^{(II)}}\begin{pmatrix}0\\ \mathcal{H}_z(k)+\sqrt{\mathcal{H}_z(k)^2}\end{pmatrix}$$
$$=\frac{1}{N^{(II)}}\begin{pmatrix}0\\ \mathcal{H}_z(k)+|\mathcal{H}_z(k)|\end{pmatrix}=\frac{1}{N^{(II)}}\begin{pmatrix}0\\ \mathcal{H}_z(k)-\mathcal{H}_z(k)\end{pmatrix}=\frac{1}{N^{(II)}}\begin{pmatrix}0\\ 0\end{pmatrix}$$

For the Hamiltonian shown above, the origin is such a point. $k_x=k_y=0$

$$\mathcal{H}_0(k)=0$$
$$\mathcal{H}_x(k)=\Delta\sin k_x=0$$
$$\mathcal{H}_y(k)=\Delta\sin k_y=0$$
$$\mathcal{H}_z(k)=-2t\cos k_x-2t\cos k_y-\mu=-4t-\mu<0$$

Therefore, we need to cut the BZ into two areas and use two different wave functions to describe the Bloch waves. They are connected by a gauge transformation

$$u_{-}^{(II)}(k)=u_{-}^{(I)}(k)e^{i\phi(k)}$$
$$\mathcal{A}_{-}^{(II)}(k)=\mathcal{A}_{-}^{(I)}(k)+\nabla_k\phi(k)$$

This is in strong analogy to the magnetic monopole case, where we need to different gauge fields.

Some comments:

- These singularities are NOT physical. If one measures any physical observables, there is no singularity anywhere in the momentum space. However. for the wavefunction and the Berry connection, which are not physical observables, there is always some singularity for this Hamiltonian.
- The location of these singularity points depends on the gauge (phase) choice. In other words, the location of the singularities has no physical meaning either.
- Only one thing about these singularities is physical, its existence. There must be some singularity points. This statement is independent of gauge choice and it tells us that the topological index is nonzero.

Let's compute the topological index for this model. For this model, there are four special points which satisfy $\mathcal{H}_x = \mathcal{H}_y = 0$. They are $\vec{k} = (0,0), \vec{k} = (\pi,\pi), \vec{k} = (0,\pi), \vec{k} = (\pi,0)$. At these four points, the values of $\mathcal{H}_z$ are: $\mathcal{H}_z = -4t - \mu, 4t - \mu, -\mu, -\mu$, respectively.

Case I: $\boldsymbol{\mu < -4t}$

If $\mu < -4t$, all the four special points has $\mathcal{H}_z > 0$. So we can use $u_-^{(II)}(k)$ for the whole Brillouin zone, and there is no singularity points.

$$u_-^{(II)}(k) = \frac{1}{N^{(I)}}\begin{pmatrix} \mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\mathcal{H}_y(k) \end{pmatrix}$$

Then we can get Berry connection

$$\mathcal{A}_-^{(II)}(k) = -i\left\langle u_-^{(II)}(k)\middle|\partial_k\middle|\left(u^{(II)}\right)_-(k)\right\rangle$$

The Berry curvature for the lower band is

$$\Omega_- = \nabla \times \mathcal{A}_-$$

Thus, the total Berry curvature (2π times the Chern number) is

$$\oiint_{BZ} dk\, \Omega_- = \oiint_{BZ} dk\, \nabla \times \mathcal{A}_- = \oint_{\partial BZ} dk\, \mathcal{A}_- = 0$$

So the Chern number is zero

$$C = \frac{1}{2\pi}\oiint_{BZ} dk\, \Omega_- = 0$$

Marginal case: $\boldsymbol{\mu = -4t}$

$\mathcal{H}_x(k) = \mathcal{H}_y(k) = \mathcal{H}_z(k) = 0$ at $\vec{k} = (0,0)$ and (π,π), the so-called Γ points.

Because the gap between the two bands is $\Delta_k = E_+ - E_- = 2\left|\vec{\mathcal{H}}(k)\right|$,

$$\Delta_k = 0 \quad at\ \vec{k} = (0,0),(\pi,\pi)$$

The gap closes at $\vec{k} = (0,0)$ and (π,π), i.e. the two energy bands touch with each other. This gives us the Dirac point. Here, the system is not an insulator, but a metal (a semi-metal). So we cannot define a topological index.

Case II: $-4t < \mu < 0$

For $-4t < \mu < 0$, $\mathcal{H}_z < 0$ at $\vec{k} = (0,0)$, and $\mathcal{H}_z > 0$ for the other three points $\vec{k} = (0,\pi),(\pi,0)$ and (π,π). Therefore, we need two wave-functions. First, we draw a small circle around the origin. Inside this small circle, which we will call region D_I, we use

$$u_-^{(I)}(k) = \frac{1}{N^{(I)}}\begin{pmatrix}\mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\mathcal{H}_y(k)\end{pmatrix}$$

Outside the circle, which we will call region D_{II}, we choose

$$u_-^{(II)}(k) = \frac{1}{N^{(I)}}\begin{pmatrix}\mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\mathcal{H}_y(k)\end{pmatrix} \times \frac{\dfrac{\mathcal{H}_z(k) + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)}}{\left|\dfrac{\mathcal{H}_z(k) + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)}\right|}$$

The wavefunctions for these two regions are connected by a gauge transformation

$$u_-^{(II)}(k) = u_-^{(I)}(k)e^{i\phi(k)}$$

And the Berry connection are related also by the same gauge transformation

$$\mathcal{A}_-^{(II)}(k) = \mathcal{A}_-^{(I)}(k) + \nabla_k\phi(k)$$

The total Berry curvature (2π times the Chern number) is

$$\begin{aligned}\iint_{BZ} dk\,\Omega_- &= \iint_{D_I} dk\nabla\times\mathcal{A}_-^{(I)} + \iint_{D_{II}} dk\nabla\times\mathcal{A}_-^{(II)} = \oint_{\partial D_I} dk\,\mathcal{A}_-^{(I)} + \oint_{\partial D_{II}} dk\,\mathcal{A}_-^{(II)} \\ &= \oint_{\partial D_I} dk\,\mathcal{A}_-^{(I)} - \oint_{\partial D_I} dk\,\mathcal{A}_-^{(II)} = \oint_{\partial D_I} dk\left(\mathcal{A}_-^{(I)} - \mathcal{A}_-^{(II)}\right) = -\oint_{\partial D_I} dk\nabla_k\phi(k) \\ &= -\int_0^{2\pi} d\theta\,\partial_\theta\phi = -[\phi(\theta = 2\pi) - \phi(\theta = 0)] = \phi(\theta = 0) - \phi(\theta = 2\pi)\end{aligned}$$

We know that $\phi(\theta = 0) - \phi(\theta = 2\pi)$ is quantized

$$\phi(\theta = 0) - \phi(\theta = 2\pi) = 2\pi n$$

Therefore, the Chern number is quantized. For the model we considered here:

$$\mathcal{H}_0(k) = 0$$

$$\mathcal{H}_x(k) = \Delta \sin k_x$$

$$\mathcal{H}_y(k) = \Delta \sin k_y$$

$$\mathcal{H}_z(k) = -2t \cos k_x - 2t \cos k_y - \mu$$

If we choose D_1 to be a very small circle with radius $k \sim 0$, then around the circle, we can expand everything as a power series of small k.

$$\mathcal{H}_x(k) = \Delta \sin k_x \approx \Delta k_x + O(k^2)$$

$$\mathcal{H}_y(k) = \Delta \sin k_y \approx \Delta k_y + O(k^2)$$

$$\mathcal{H}_z(k) = -2t \cos k_x - 2t \cos k_y - \mu = -4t - \mu + O(k^2)$$

$$e^{i\phi(k)} = \frac{\dfrac{\mathcal{H}_z(k) + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)}}{\left|\dfrac{\mathcal{H}_z(k) + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)}\right|} = \frac{\dfrac{1}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)}}{\left|\dfrac{1}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)}\right|} = \frac{\left|\mathcal{H}_x(k) + i\mathcal{H}_y(k)\right|}{\mathcal{H}_x(k) + i\mathcal{H}_y(k)} = \frac{\left|\Delta k_x + i\Delta k_y\right|}{\Delta k_x + i\Delta k_y}$$

$$= \frac{\left|k_x + ik_y\right|}{k_x + ik_y} = \frac{\left|ke^{i\theta}\right|}{ke^{i\theta}} = \frac{1}{e^{i\theta}} = e^{-i\theta}$$

Here, we transfer $k_x + ik_y$ into polar coordinate, which is $ke^{i\theta}$. This result tells us that

$$\phi(k) = -\theta$$

Therefore,

$$\oiint_{BZ} dk\, \Omega_- = \phi(\theta = 0) - \phi(\theta = 2\pi) = 0 - (-2\pi) = 2\pi$$

So,

$$C = \frac{1}{2\pi} \oiint_{BZ} dk\, \Omega_- = 1$$

Marginal case: $\mu = 0$

The gap closes at $\vec{k} = (0, \pi)$ and $(\pi, 0)$, two inequivalent so-called *X* points. The system is not an insulator, so we cannot define the Chern number.

Case III: $0 < \mu < 4t$

For $0 < \mu < 4t$, $\mathcal{H}_z > 0$ at $\vec{k} = (\pi, \pi)$ and $\mathcal{H}_z < 0$ for the other three points. Here, we can draw a small circle centered at (π, π) to cut the system into two parts. Inside the circle, near (π, π), we use u^{II} and outside the circle, near (0, 0) we use u^{I}. Same as case II, we get a topological insulator with $C = -1$.

Marginal case: $\mu = 4t$

The gap closes at $\vec{k} = (\pm\pi, \pm\pi)$, the so-called *M* point. Not an insulator.

Case IV: $\mu > 4t$

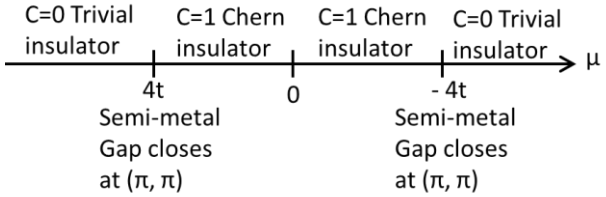
All the four special points has $\mathcal{H}_z < 0$. So we just use u^{I} for the whole BZ. No singularity, and thus $C = 0$.

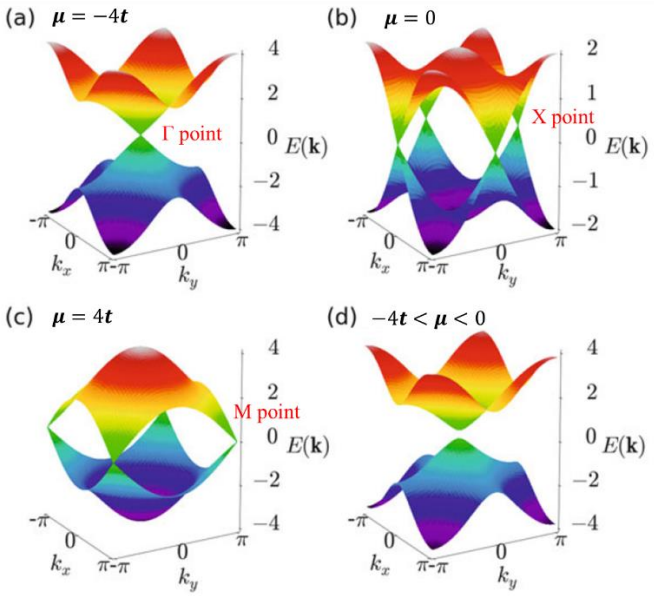
The top band?

The top band has the opposite Chern number $C_+ = -C_-$. This is because for any tight-binding models, the total Chern number for all the bands is always 0. So here, we have $C_+ + C_- = 0$.

Summary

- This model has four phases. Two topological phases with $C = +/-1$ and two trivial insulator phase with $C = 0$.
- A topological phase and a trivial insulator phase are always separated by a phase transition, which is known as a topological phase transition.
    - Across the topological phase transition, the topological index changes its value
    - **Across a topological transition, the insulating gap closes and then reopens (generically true)**
- Gap closing is the necessary condition for a topological transition, but it is not sufficient. One may close and reopen the gap without changing the topological index. e.g. the $\mu = 0$ point here.





This is simple to show, since the gap closing requires $\Delta(k) = 0$ at some **k**. In the vicinity of a gap closing point, called Dirac point, the dispersion relation has the shape of a Dirac cone. For all other values of $\mu \neq -4t, 0, 4t$, the spectrum is gapped, and thus it makes sense to investigate the topological properties of the system.

Although we calculated the Chern number of the corresponding, we show the graphical way to calculate the Chern number of the QWZ model.

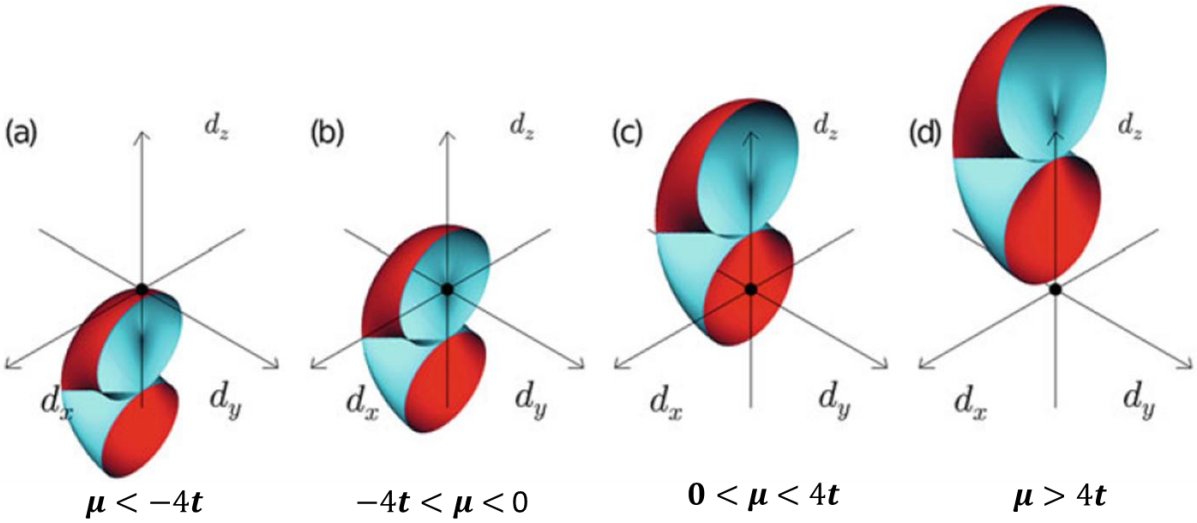
Refer to the eigenvalues of $\mathcal{H}$ are

$$E_{\pm} = \mathcal{H}_0(k) \pm |\mathcal{H}(k)| = \mathcal{H}_0(k) \pm \sqrt{\mathcal{H}_x(k)^2 + \mathcal{H}_y(k)^2 + \mathcal{H}_z(k)^2}$$

Usually the value of $\mathcal{H}_0(k)$ is set to zero since this energy offset does not change the topological property of the system and if you do not concern the total energy of the system. Then we usually denote

$$E_{\pm} = \pm|\mathcal{H}(k)| = \pm|\mathbf{d}(d_x, d_y)|$$

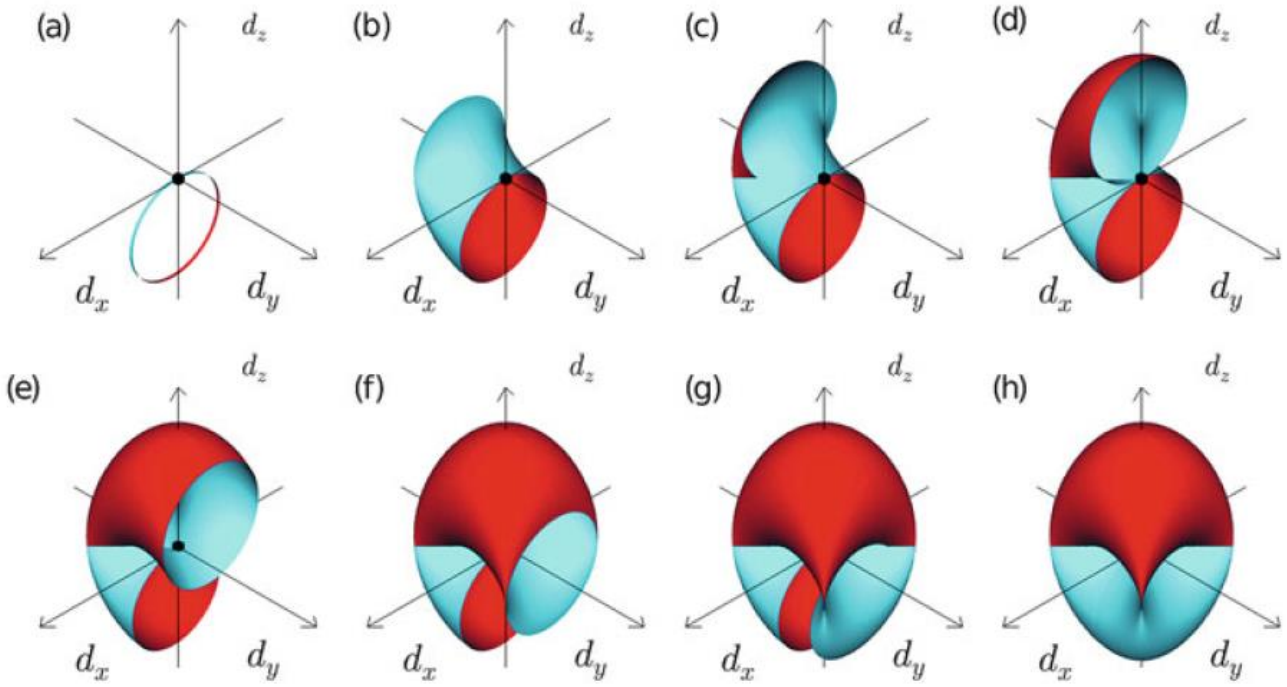
Then we can simply count how many times the torus of the image of the Brillouin zone in the space of **d** contains the origin. To get some feeling about the not so trivial geometry of the torus, it is instructive to follow a gradual sweep of the Brillouin zone. The parameter μ shifts the whole torus along the d_z direction, thus as we tune it we also control whether the origin is contained inside it or not. For the QWZ model three situations can occur as depicted as follows:



The torus $\mathbf{d}(\mathbf{k})$ of the QWZ model for different values of μ. For clarity only the image of half of the Brillouin zone is shown. In (a) and (d) the torus does not contain the origin hence C=0. In (b), taking an infinite line from the origin along the positive z axis, we hit the blue side of the torus once hence C=-1. In (c), taking the infinite line in the negative z direction, we hit the red side of the torus thus C=1.

It can happen that the torus does not contain the origin, as in (a) and (d), and the Chern number is 0. This is the case for $|\mu| > 4t$. It can also happen that the origin is in the inside of the torus: a line from the origin to infinity will then inevitably pierce the torus. The first piercing can be from the blue side (outside) of the surface as in (b), or from the red side (inside) as in (c).

If μ happens to take $-4t, 4t, 0$, then we have the origin sitting on the surface of the torus. As an example, below we show when $\mu = 0$:



The surface $\mathbf{d}(\mathbf{k})$ for the QWZ model as $\mathbf{k}$ sweeps through the whole Brillouin zone. To illustrate how this surface is a torus the sweeping is done gradually with $\mu = 0$. In (a) the image of the $k_y = -\pi$ line is depicted. In (b) the image for the region $k_y = -\pi \ldots -0.5\pi$, in (c) $k_y = -\pi \ldots -0.25\pi$, in (d) $k_y = -\pi \ldots -0$, in (e) $k_y = -\pi \ldots 0.25\pi$, in (f) $k_y = -\pi \ldots 0.5\pi$, in (g) $k_y = -\pi \ldots 0.75\pi$ and finally in (h) the image of the whole Brillouin zone is depicted and the torus is closed. Since the torus in these cases do not contain the origin, the Chern numbers are 0.